



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:45 AM UTC

PDB ID : 2USH / pdb_00002ush
Title : 5'-NUCLEOTIDASE FROM E. COLI
Authors : Knofel, T.; Strater, N.
Deposited on : 1998-09-24
Resolution : 2.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

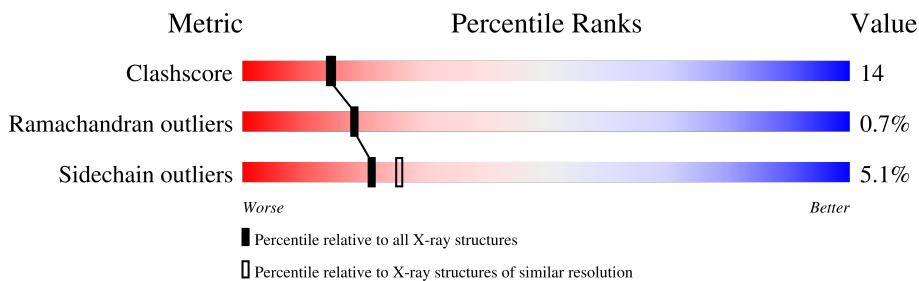
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	550	 63% 25% • 8%
1	B	550	 63% 29% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8180 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

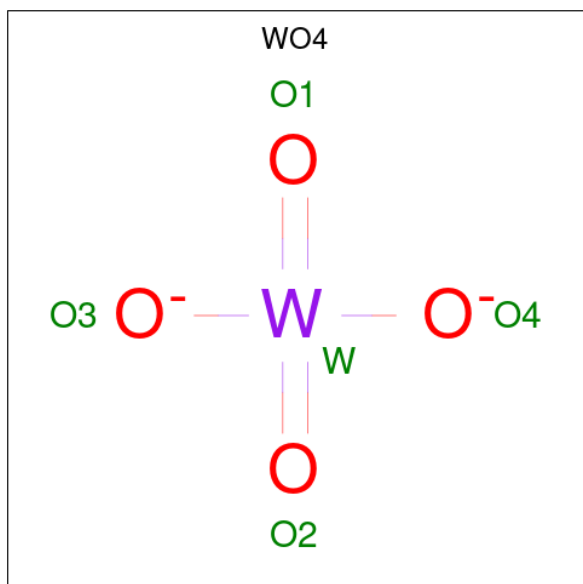
- Molecule 1 is a protein called 5'-NUCLEOTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	506	3950	2499	678	756	17	0	0	0
1	B	520	4064	2570	696	781	17	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Zn	0	0
			5	5		
2	B	4	Total	Zn	0	0
			4	4		

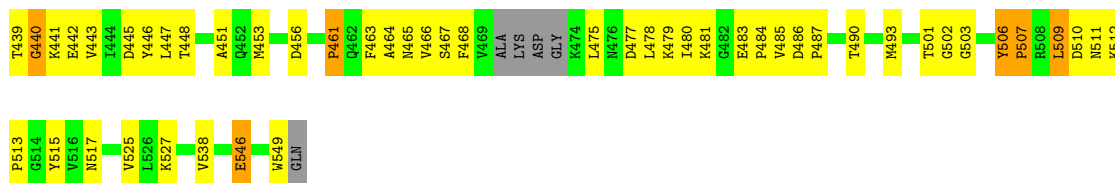
- Molecule 3 is TUNGSTATE(VI)ION (CCD ID: WO4) (formula: O₄W).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	W	0	0
			5	4	1		
3	A	1	Total	O	W	0	0
			5	4	1		
3	B	1	Total	O	W	0	0
			5	4	1		
3	B	1	Total	O	W	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	70	Total	O	0	0
			70	70		



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.21Å 116.29Å 132.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.22	Depositor
% Data completeness (in resolution range)	98.2 (8.00-2.22)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.198 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8180	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: WO4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.75	1/4032 (0.0%)	1.28	32/5451 (0.6%)
1	B	0.74	0/4151	1.22	28/5617 (0.5%)
All	All	0.75	1/8183 (0.0%)	1.25	60/11068 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	MET	SD-CE	-5.17	1.66	1.79

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	LEU	N-CA-C	-11.46	99.31	113.97
1	B	179	GLY	N-CA-C	-10.19	89.03	113.18
1	A	315	ILE	N-CA-C	9.52	116.22	107.56
1	A	546	GLU	N-CA-C	9.37	122.48	111.71
1	A	118	GLU	N-CA-C	-8.35	103.08	113.18
1	A	509	LEU	N-CA-C	-8.22	103.45	113.97
1	A	483	GLU	CA-C-N	7.99	128.46	119.92
1	A	483	GLU	C-N-CA	7.99	128.46	119.92
1	A	256	PRO	N-CA-C	-7.98	96.03	112.47
1	A	43	HIS	N-CA-C	7.45	121.67	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	TYR	CA-C-N	7.38	127.80	119.83
1	A	506	TYR	C-N-CA	7.38	127.80	119.83
1	A	121	ASN	CA-C-N	7.28	127.25	119.76
1	A	121	ASN	C-N-CA	7.28	127.25	119.76
1	B	256	PRO	N-CA-C	-7.13	97.79	112.47
1	A	291	TRP	N-CA-C	7.08	121.50	112.86
1	B	506	TYR	CA-C-N	6.96	127.00	119.90
1	B	506	TYR	C-N-CA	6.96	127.00	119.90
1	B	314	LEU	N-CA-C	-6.67	96.35	108.02
1	A	485	VAL	CB-CA-C	-6.59	104.81	111.80
1	A	85	ILE	N-CA-C	-6.56	104.63	111.58
1	B	372	GLU	N-CA-C	6.53	118.55	109.15
1	B	362	VAL	N-CA-C	6.50	118.05	109.21
1	B	250	GLY	N-CA-C	6.46	121.42	112.57
1	B	183	TYR	N-CA-C	6.34	120.31	111.56
1	A	461	PRO	N-CA-C	6.26	120.75	110.55
1	B	255	ASP	CB-CA-C	-6.19	98.74	109.32
1	A	250	GLY	N-CA-C	6.13	120.96	112.57
1	B	267	VAL	N-CA-C	6.03	116.81	110.72
1	A	376	ASP	N-CA-C	-5.97	105.84	113.01
1	A	276	LYS	CA-C-N	5.97	126.31	119.92
1	A	276	LYS	C-N-CA	5.97	126.31	119.92
1	A	485	VAL	N-CA-C	5.94	115.81	107.37
1	A	215	ALA	N-CA-C	-5.76	99.35	108.73
1	B	160	ARG	N-CA-C	-5.76	98.90	108.34
1	A	429	PHE	N-CA-C	5.66	120.18	113.16
1	B	483	GLU	CA-C-N	5.62	125.53	119.85
1	B	483	GLU	C-N-CA	5.62	125.53	119.85
1	B	137	LEU	N-CA-C	-5.58	99.43	108.52
1	B	503	GLY	N-CA-C	-5.57	105.52	111.93
1	A	385	MET	N-CA-C	-5.57	105.29	111.36
1	B	118	GLU	N-CA-C	-5.55	106.35	113.01
1	A	420	TYR	N-CA-C	-5.49	105.46	111.82
1	B	461	PRO	N-CA-C	5.48	120.83	111.68
1	B	43	HIS	N-CA-C	5.46	118.87	111.17
1	A	372	GLU	N-CA-C	5.46	117.01	109.15
1	B	260	ALA	N-CA-C	-5.46	106.75	113.41
1	A	255	ASP	CB-CA-C	-5.37	100.74	108.84
1	A	141	ASN	N-CA-C	5.36	119.52	112.92
1	B	291	TRP	N-CA-C	5.34	122.17	110.80
1	A	89	VAL	CA-C-N	5.30	124.76	119.24
1	A	89	VAL	C-N-CA	5.30	124.76	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	LYS	N-CA-C	5.28	117.72	111.33
1	B	215	ALA	N-CA-C	-5.16	100.32	108.73
1	A	391	ALA	N-CA-C	-5.13	105.76	111.36
1	B	98	GLU	CA-C-N	-5.13	113.64	119.28
1	B	98	GLU	C-N-CA	-5.13	113.64	119.28
1	A	163	LEU	N-CA-C	5.12	118.29	110.20
1	B	376	ASP	CB-CA-C	-5.07	101.25	110.63
1	B	253	SER	N-CA-C	-5.00	106.44	112.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	515	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3950	0	3880	108	0
1	B	4064	0	3985	116	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	67	0	0	2	0
4	B	70	0	0	3	0
All	All	8180	0	7865	224	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:H	1:A:422:ASN:HD22	1.06	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:O	1:A:177:LYS:HG3	1.64	0.97
1:B:368:ASN:HD21	1:B:538:VAL:H	1.11	0.92
1:A:463:PHE:HB3	1:A:466:VAL:CG1	2.03	0.89
1:A:441:LYS:HE2	1:A:445:ASP:OD2	1.73	0.89
1:A:419:SER:H	1:A:422:ASN:ND2	1.71	0.89
1:B:453:MET:HE3	1:B:453:MET:HA	1.57	0.87
1:A:479:LYS:HD3	1:A:482:GLY:O	1.78	0.83
1:A:153:LYS:HD3	1:A:153:LYS:N	1.95	0.81
1:A:50:GLU:CD	1:A:50:GLU:H	1.90	0.80
1:A:153:LYS:CD	1:A:153:LYS:H	1.96	0.79
1:B:477:ASP:OD1	1:B:479:LYS:HE3	1.82	0.79
1:A:153:LYS:H	1:A:153:LYS:CE	1.97	0.77
1:A:479:LYS:HE2	1:A:484:PRO:HG3	1.65	0.77
1:B:180:ASN:OD1	1:B:182:GLU:HB3	1.83	0.77
1:B:180:ASN:CG	1:B:182:GLU:HB3	2.10	0.77
1:B:463:PHE:HB3	1:B:466:VAL:HG22	1.67	0.75
1:B:175:THR:O	1:B:179:GLY:HA3	1.86	0.74
1:B:323:VAL:O	1:B:330:SER:HA	1.87	0.74
1:A:372:GLU:HG2	1:A:377:LYS:HD3	1.70	0.72
1:A:467:SER:HB3	1:A:546:GLU:HB2	1.69	0.72
1:B:419:SER:H	1:B:422:ASN:ND2	1.90	0.70
1:A:153:LYS:HD3	1:A:153:LYS:H	1.53	0.69
1:B:91:GLU:OE1	1:B:91:GLU:N	2.24	0.69
1:B:122:PRO:HB2	1:B:124:THR:HG22	1.75	0.69
1:A:419:SER:N	1:A:422:ASN:HD22	1.88	0.68
1:A:153:LYS:N	1:A:153:LYS:CD	2.55	0.68
1:B:368:ASN:ND2	1:B:538:VAL:H	1.89	0.67
1:A:188:GLU:OE1	1:A:190:ARG:NH1	2.29	0.65
1:B:368:ASN:HD21	1:B:538:VAL:HG22	1.61	0.65
1:A:470:ALA:HB3	1:A:549:TRP:CD1	2.31	0.65
1:A:546:GLU:CD	1:A:546:GLU:H	2.04	0.65
1:B:511:ASN:OD1	1:B:512:LYS:HE3	1.98	0.64
1:A:321:LYS:HB3	1:A:335:TYR:CZ	2.32	0.64
1:B:368:ASN:ND2	1:B:538:VAL:HG22	2.13	0.64
1:B:502:GLY:HA2	1:B:506:TYR:O	1.98	0.64
1:B:451:ALA:O	1:B:549:TRP:CZ3	2.51	0.64
1:B:350:SER:HB2	1:B:351:PRO:HD3	1.80	0.63
1:A:463:PHE:HB3	1:A:466:VAL:HG13	1.81	0.63
1:B:222:ASP:OD1	1:B:265:LYS:HE2	1.99	0.62
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.64	0.62
1:A:432:VAL:HG22	1:A:521:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:O	1:A:177:LYS:CG	2.45	0.62
1:B:303:ARG:HH11	1:B:303:ARG:CG	2.12	0.61
1:B:425:LYS:NZ	1:B:425:LYS:HB3	2.15	0.61
1:A:441:LYS:HE2	1:A:445:ASP:CG	2.25	0.61
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.65	0.61
1:A:468:PHE:H	1:A:547:VAL:HA	1.66	0.60
1:B:146:SER:N	1:B:186:ASP:OD1	2.34	0.60
1:B:99:PRO:HB3	1:B:352:PHE:CG	2.37	0.59
1:B:438:MET:HE2	1:B:442:GLU:HB3	1.85	0.59
1:A:493:MET:CE	1:A:509:LEU:HD11	2.34	0.58
1:B:174:ASP:OD1	1:B:177:LYS:HE3	2.04	0.58
1:A:257:VAL:HG23	1:A:287:GLN:HB3	1.86	0.57
1:A:241:PRO:HG2	1:A:244:SER:HB3	1.87	0.57
1:A:434:VAL:HG12	1:A:517:ASN:HA	1.87	0.57
1:A:57:ALA:HA	1:A:345:MET:HG2	1.86	0.57
1:A:256:PRO:O	1:A:256:PRO:HG2	2.05	0.57
1:B:180:ASN:ND2	1:B:182:GLU:HB3	2.20	0.57
1:B:419:SER:H	1:B:422:ASN:HD22	1.53	0.57
1:B:448:THR:HA	1:B:475:LEU:HD11	1.86	0.57
1:A:27:GLU:OE1	1:A:162:ASP:OD2	2.23	0.56
1:A:153:LYS:H	1:A:153:LYS:HE2	1.69	0.56
1:B:465:ASN:N	1:B:465:ASN:HD22	2.03	0.56
1:A:190:ARG:HG2	1:A:190:ARG:HH11	1.70	0.56
1:B:226:HIS:CE1	1:B:231:PRO:HG3	2.40	0.56
1:A:493:MET:HE1	1:A:509:LEU:HD11	1.86	0.56
1:B:257:VAL:HG23	1:B:287:GLN:HB3	1.88	0.56
1:A:440:GLY:O	1:A:443:VAL:HG22	2.05	0.56
1:A:43:HIS:CE1	1:A:84:ASP:HB3	2.40	0.55
1:B:463:PHE:HB3	1:B:466:VAL:CG2	2.34	0.55
1:A:467:SER:CB	1:A:546:GLU:HB2	2.35	0.55
1:A:176:ALA:C	1:A:177:LYS:HG3	2.29	0.55
1:B:463:PHE:CD1	1:B:466:VAL:HG21	2.40	0.55
1:A:223:ASN:HB2	1:A:263:ASN:HB3	1.87	0.55
1:B:325:TRP:N	1:B:329:LYS:O	2.29	0.55
1:B:443:VAL:O	1:B:447:LEU:HG	2.07	0.54
1:B:102:ARG:HG2	1:B:102:ARG:HH11	1.71	0.54
1:A:91:GLU:OE1	1:A:91:GLU:N	2.38	0.54
1:A:372:GLU:CG	1:A:377:LYS:HD3	2.37	0.54
1:A:32:TYR:CG	1:A:163:LEU:HD21	2.43	0.54
1:A:144:GLN:HB2	1:A:151:LEU:HD21	1.89	0.54
1:B:180:ASN:O	1:B:182:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:O	1:B:67:ARG:HG3	2.09	0.53
1:B:256:PRO:O	1:B:256:PRO:HG2	2.09	0.53
1:B:180:ASN:C	1:B:182:GLU:N	2.65	0.53
1:A:288:ALA:O	1:A:289:HIS:HB3	2.07	0.52
1:B:125:VAL:O	1:B:128:GLN:HB3	2.10	0.52
1:B:480:ILE:O	1:B:481:LYS:HB2	2.08	0.52
1:B:271:PRO:HG3	1:B:294:TYR:OH	2.10	0.52
1:A:479:LYS:HG2	1:A:484:PRO:HA	1.92	0.51
1:A:300:PHE:CG	1:A:307:MET:HE3	2.45	0.51
1:B:69:GLU:HG3	1:B:70:VAL:N	2.25	0.51
1:A:103:GLY:O	1:A:345:MET:HE1	2.10	0.51
1:B:321:LYS:HB3	1:B:335:TYR:CZ	2.45	0.50
1:B:380:PHE:CE2	1:B:456:ASP:HB2	2.47	0.50
1:B:368:ASN:HD22	1:B:368:ASN:H	1.58	0.50
1:B:511:ASN:O	1:B:512:LYS:HD3	2.11	0.50
1:B:546:GLU:H	1:B:546:GLU:CD	2.18	0.50
1:B:468:PHE:CD1	1:B:468:PHE:C	2.90	0.50
1:A:163:LEU:N	1:A:163:LEU:HD22	2.27	0.49
1:B:368:ASN:HD22	1:B:368:ASN:N	2.10	0.49
1:B:327:ASP:OD1	1:B:327:ASP:C	2.55	0.49
1:B:451:ALA:O	1:B:549:TRP:HZ3	1.95	0.49
1:A:321:LYS:O	1:A:332:ARG:HA	2.12	0.49
1:A:420:TYR:O	1:A:423:VAL:HG22	2.13	0.49
1:A:468:PHE:O	1:A:548:SER:N	2.45	0.49
1:B:367:THR:HG23	1:B:415:ALA:HA	1.94	0.49
1:A:271:PRO:HG2	1:A:335:TYR:CD2	2.47	0.49
1:A:334:LEU:CD1	1:A:338:GLU:HB2	2.43	0.49
1:B:433:VAL:HG21	1:B:525:VAL:HG21	1.93	0.49
1:A:410:ARG:HG3	1:A:428:PRO:HD2	1.95	0.49
1:B:73:GLU:OE2	4:B:815:HOH:O	2.20	0.49
1:A:410:ARG:HG3	1:A:428:PRO:CD	2.43	0.48
1:B:180:ASN:C	1:B:182:GLU:H	2.20	0.48
1:B:381:VAL:HG22	1:B:382:GLN:N	2.27	0.48
1:B:102:ARG:HG2	1:B:102:ARG:NH1	2.27	0.48
1:B:143:TYR:CE2	1:B:190:ARG:HD2	2.49	0.48
1:B:418:ILE:HA	1:B:422:ASN:ND2	2.28	0.48
1:A:411:ASP:OD1	1:A:412:SER:N	2.44	0.48
1:B:467:SER:HA	1:B:546:GLU:O	2.13	0.48
1:A:59:GLN:NE2	1:A:109:TYR:OH	2.47	0.48
1:A:95:GLN:NE2	1:A:355:LYS:HD3	2.29	0.48
1:A:353:GLN:O	1:A:357:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:MET:CE	1:B:509:LEU:HD11	2.44	0.47
1:A:421:LYS:HE2	1:A:425:LYS:NZ	2.29	0.47
1:A:196:ALA:O	1:A:200:ILE:HG13	2.13	0.47
1:B:441:LYS:NZ	1:B:445:ASP:OD1	2.45	0.47
1:A:463:PHE:HB3	1:A:466:VAL:HG11	1.91	0.47
1:A:470:ALA:N	1:A:548:SER:O	2.41	0.47
1:A:185:THR:O	1:A:186:ASP:HB3	2.15	0.47
1:A:517:ASN:OD1	1:A:517:ASN:C	2.58	0.47
1:B:446:TYR:CE1	1:B:507:PRO:HB2	2.50	0.47
1:A:380:PHE:CZ	1:A:456:ASP:HA	2.49	0.47
1:B:323:VAL:O	1:B:331:GLU:N	2.43	0.46
1:A:353:GLN:NE2	1:A:353:GLN:HA	2.30	0.46
1:B:324:THR:HA	1:B:330:SER:HA	1.97	0.46
1:B:364:ILE:HD12	1:B:527:LYS:HG3	1.97	0.46
1:B:144:GLN:O	1:B:148:GLY:N	2.48	0.46
1:A:468:PHE:C	1:A:468:PHE:CD1	2.93	0.46
1:A:403:VAL:HG12	1:A:404:MET:N	2.30	0.46
1:B:325:TRP:HD1	1:B:329:LYS:HG2	1.81	0.46
1:A:435:TYR:CZ	1:A:516:VAL:HG21	2.51	0.46
1:B:325:TRP:HD1	1:B:329:LYS:CG	2.30	0.45
1:A:259:MET:HG2	1:A:276:LYS:O	2.17	0.45
1:A:236:MET:CE	1:A:248:ILE:HD13	2.47	0.45
1:B:425:LYS:HB3	1:B:425:LYS:HZ2	1.82	0.45
1:A:353:GLN:HA	1:A:353:GLN:HE21	1.81	0.45
1:A:310:VAL:O	1:A:311:ASN:HB2	2.17	0.45
1:B:443:VAL:CG2	1:B:485:VAL:HG11	2.47	0.45
1:B:223:ASN:HB2	1:B:263:ASN:HB3	1.99	0.45
1:B:239:ALA:HB2	4:B:911:HOH:O	2.16	0.45
1:B:439:THR:HA	1:B:490:THR:HA	1.99	0.45
1:A:419:SER:N	1:A:422:ASN:ND2	2.54	0.44
1:B:157:LEU:HD13	1:B:166:ALA:HB2	1.99	0.44
1:A:26:TYR:HB2	1:A:32:TYR:CE1	2.53	0.44
1:B:28:GLN:HG3	1:B:304:ASN:OD1	2.18	0.44
1:B:141:ASN:ND2	1:B:192:PRO:HG3	2.32	0.44
1:B:440:GLY:HA3	1:B:486:ASP:O	2.18	0.44
1:A:516:VAL:O	1:A:516:VAL:CG2	2.64	0.44
1:B:298:ALA:HB1	1:B:309:MET:HE2	2.00	0.44
1:A:463:PHE:CD1	1:A:466:VAL:HG11	2.54	0.43
1:A:190:ARG:HH11	1:A:190:ARG:CG	2.32	0.43
1:B:32:TYR:O	1:B:301:GLU:HA	2.18	0.43
1:B:438:MET:O	1:B:490:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:CD1	1:B:338:GLU:HB2	2.49	0.43
1:B:302:PHE:HA	1:B:306:GLU:O	2.19	0.43
1:B:368:ASN:HD21	1:B:538:VAL:N	1.95	0.43
1:A:118:GLU:HB3	1:A:126:LEU:HD13	2.01	0.43
1:A:251:GLY:O	1:A:252:HIS:HB3	2.19	0.43
1:B:190:ARG:O	1:B:191:LYS:C	2.62	0.43
1:A:27:GLU:CD	1:A:162:ASP:OD2	2.62	0.42
1:A:48:ARG:NH1	1:A:341:GLU:OE1	2.52	0.42
1:B:374:ASP:O	1:B:378:VAL:HG22	2.19	0.42
1:B:501:THR:HA	1:B:510:ASP:HB2	1.99	0.42
1:A:271:PRO:HG2	1:A:335:TYR:CE2	2.54	0.42
1:B:59:GLN:NE2	1:B:109:TYR:OH	2.50	0.42
1:A:357:LYS:HD2	1:A:357:LYS:HA	1.85	0.42
1:B:144:GLN:HB2	1:B:151:LEU:HD21	2.01	0.42
1:A:350:SER:N	1:A:351:PRO:CD	2.82	0.42
1:A:483:GLU:HA	1:A:484:PRO:HD3	1.75	0.42
1:A:341:GLU:OE1	1:A:346:ILE:HD11	2.20	0.42
1:B:334:LEU:HD11	1:B:338:GLU:HB2	2.02	0.42
1:A:206:THR:HG22	1:A:207:GLU:N	2.34	0.42
1:B:28:GLN:HG2	1:B:29:ASP:N	2.33	0.42
1:B:216:THR:HG21	1:B:236:MET:HE1	2.02	0.42
1:A:99:PRO:HB3	1:A:352:PHE:CG	2.55	0.42
1:A:217:HIS:CD2	1:A:252:HIS:HB2	2.54	0.42
1:B:464:ALA:O	1:B:465:ASN:HB2	2.19	0.42
1:A:455:PRO:O	1:A:456:ASP:HB3	2.20	0.41
1:B:438:MET:O	1:B:490:THR:HG23	2.20	0.41
1:B:467:SER:O	1:B:478:LEU:HA	2.20	0.41
1:A:137:LEU:O	1:A:153:LYS:CE	2.68	0.41
1:A:154:PRO:HG2	1:A:155:TRP:CE3	2.56	0.41
1:A:469:VAL:HA	1:A:548:SER:O	2.20	0.41
1:A:470:ALA:O	1:A:471:LYS:HG3	2.20	0.41
1:B:95:GLN:OE1	1:B:355:LYS:HD3	2.21	0.41
1:A:440:GLY:O	1:A:444:ILE:HG13	2.20	0.41
1:A:522:ASP:OD1	1:A:523:ALA:N	2.52	0.41
1:B:192:PRO:HD2	4:B:926:HOH:O	2.19	0.41
1:B:448:THR:HA	1:B:475:LEU:CD1	2.49	0.41
1:B:465:ASN:N	1:B:465:ASN:ND2	2.68	0.41
1:A:467:SER:HA	1:A:546:GLU:O	2.20	0.41
1:B:43:HIS:O	1:B:45:HIS:CD2	2.74	0.41
1:B:265:LYS:HE2	1:B:265:LYS:HB3	1.84	0.41
1:A:367:THR:HG23	1:A:415:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LEU:HB3	1:B:421:LYS:HG3	2.03	0.41
1:B:453:MET:HA	1:B:453:MET:CE	2.40	0.41
1:A:59:GLN:O	1:A:63:VAL:HG23	2.20	0.41
1:A:435:TYR:CE2	1:A:516:VAL:CG2	3.03	0.41
1:B:325:TRP:CD1	1:B:329:LYS:HD3	2.56	0.41
1:A:399:ALA:HA	1:A:492:ARG:HG2	2.02	0.41
1:B:28:GLN:CG	1:B:29:ASP:N	2.83	0.41
1:B:199:VAL:O	1:B:203:LEU:HD23	2.20	0.41
1:A:526:LEU:HD22	1:A:530:ILE:CD1	2.52	0.40
1:A:188:GLU:HG3	4:A:937:HOH:O	2.20	0.40
1:B:122:PRO:HB2	1:B:124:THR:CG2	2.47	0.40
1:B:434:VAL:HG12	1:B:517:ASN:HA	2.02	0.40
1:A:60:LYS:HD2	1:A:106:LEU:HG	2.03	0.40
1:A:220:HIS:HA	4:A:850:HOH:O	2.21	0.40
1:B:212:ILE:HG22	1:B:245:LEU:HD23	2.03	0.40
1:B:493:MET:HE2	1:B:509:LEU:HD11	2.03	0.40
1:B:241:PRO:HB2	1:B:244:SER:HB3	2.02	0.40
1:B:373:GLY:HA3	1:B:411:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/550 (90%)	469 (94%)	25 (5%)	4 (1%)	16	15
1	B	516/550 (94%)	481 (93%)	32 (6%)	3 (1%)	21	22
All	All	1014/1100 (92%)	950 (94%)	57 (6%)	7 (1%)	18	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	TYR
1	A	146	SER
1	A	289	HIS
1	B	54	TYR
1	A	87	THR
1	B	289	HIS
1	B	440	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/452 (92%)	395 (95%)	22 (5%)	20	24
1	B	430/452 (95%)	409 (95%)	21 (5%)	22	27
All	All	847/904 (94%)	804 (95%)	43 (5%)	21	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	94	LEU
1	A	122	PRO
1	A	136	PRO
1	A	154	PRO
1	A	192	PRO
1	A	231	PRO
1	A	256	PRO
1	A	274	PRO
1	A	277	PRO
1	A	337	PRO
1	A	351	PRO
1	A	428	PRO
1	A	461	PRO
1	A	484	PRO
1	A	487	PRO
1	A	507	PRO

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Mol	Chain	Res	Type
1	A	513	PRO
1	A	516	VAL
1	A	526	LEU
1	A	535	PRO
1	A	546	GLU
1	B	90	PRO
1	B	122	PRO
1	B	136	PRO
1	B	154	PRO
1	B	181	PRO
1	B	209	PRO
1	B	231	PRO
1	B	241	PRO
1	B	271	PRO
1	B	274	PRO
1	B	303	ARG
1	B	337	PRO
1	B	351	PRO
1	B	368	ASN
1	B	428	PRO
1	B	461	PRO
1	B	484	PRO
1	B	487	PRO
1	B	507	PRO
1	B	513	PRO
1	B	546	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	128	GLN
1	A	229	ASN
1	A	266	GLN
1	A	313	GLN
1	A	344	GLN
1	A	353	GLN
1	A	354	ASN
1	A	393	GLN
1	A	422	ASN
1	A	427	GLN
1	A	431	ASN

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Mol	Chain	Res	Type
1	B	59	GLN
1	B	263	ASN
1	B	279	GLN
1	B	354	ASN
1	B	359	GLN
1	B	368	ASN
1	B	393	GLN
1	B	422	ASN
1	B	427	GLN
1	B	452	GLN
1	B	465	ASN
1	B	499	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	WO4	B	701	-	2,4,4	0.72	0	-		
3	WO4	B	704	3	2,4,4	0.45	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	WO4	A	703	2,3	2,4,4	0.72	0	-		
3	WO4	A	702	3	2,4,4	0.56	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.